FDS v5 - Multi-step Combustion and Other Code Improvements

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FIRE SCIENCE & ENGINEERING

Overview

- 2 and 3 parameter mixture fraction and related code changes
- Validation examples
- Misc. new features

Two-parameter Mixture Fraction

$$Z_1 + Z_2 = Y_{CH_4} + \frac{W_{CH_4}}{W_{CO_2}} Y_{CO2}$$

Mass of unburned fuel

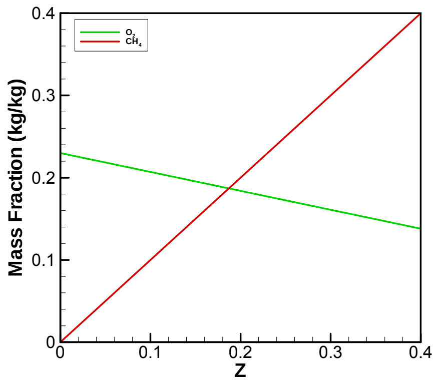
Mass of fuel converted to CO_2 and associated products

$$Z_1 + Z_2 = Z$$

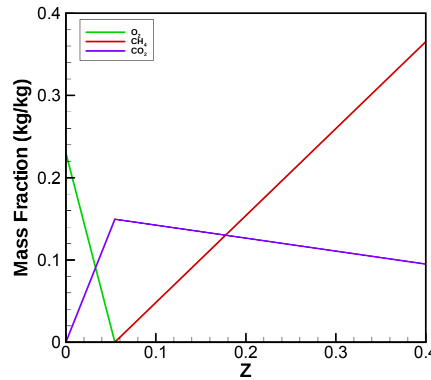
Two-parameter State Relations

CH$_4$ to CH$_4$ | CH$_4$ to CO$_2$ | Actual

(1-F) x



+ F x



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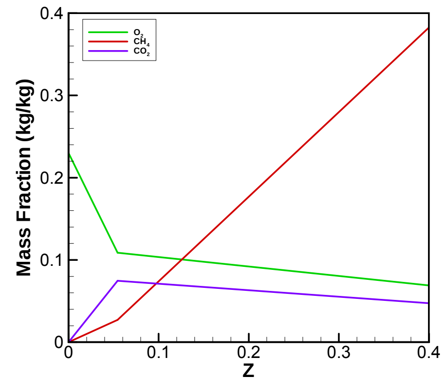
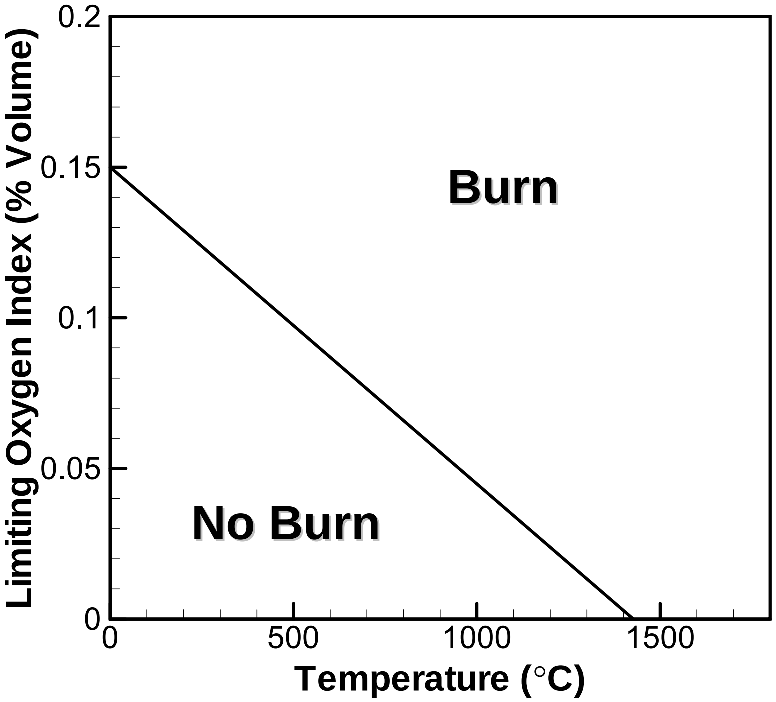


F = Degree of completion of combustion (F=0.5)
for clarity, N$_2$ and H$_2$O have been omitted

Reaction Kinetics

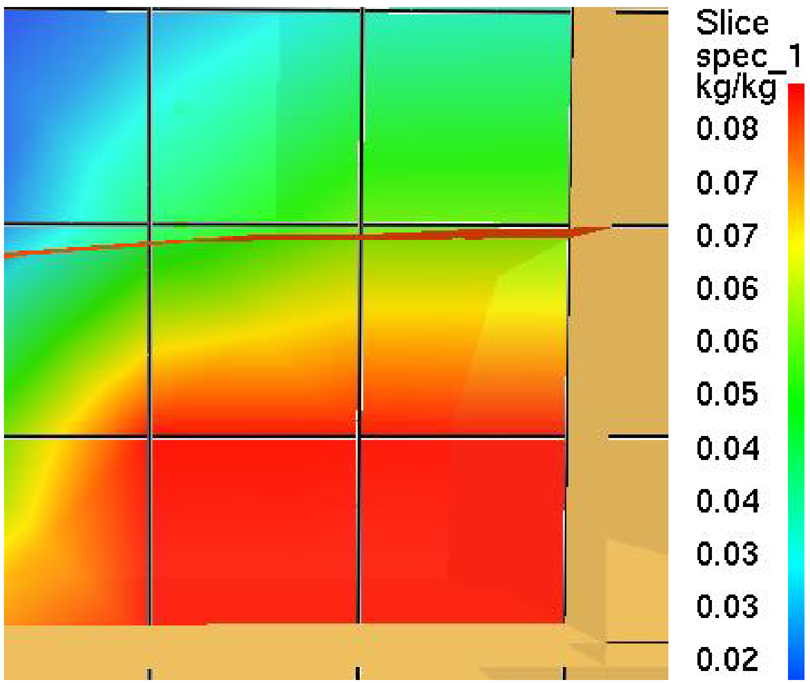
- Reaction is infinitely fast
- Reaction prohibited if the oxygen content in the current cell and all adjacent cells is below a critical value for the cell's temperature
- User can disable



Combustion

- FDS v4 – Gradient of Z at Z_F Surface
  - Did not always get correct HRR for well ventilated fires
  - Unrealistic volumetric HRR
  - Cannot turn off product formation

- FDS v5 – Fuel + $O_2 \rightarrow$ Products
  - Guarantee the HRR for well ventilated fires
  - Extinction means no product formation
  - Lesser issue of unrealistic volumetric HRR



Three-parameter Mixture Fraction

$$Z_1 + Z_2 + Z_3 = Y_{CH_4} + \frac{W_{CH_4}}{W_{CO}} Y_{CO} + \frac{W_{CH_4}}{W_{CO_2}} Y_{CO2}$$

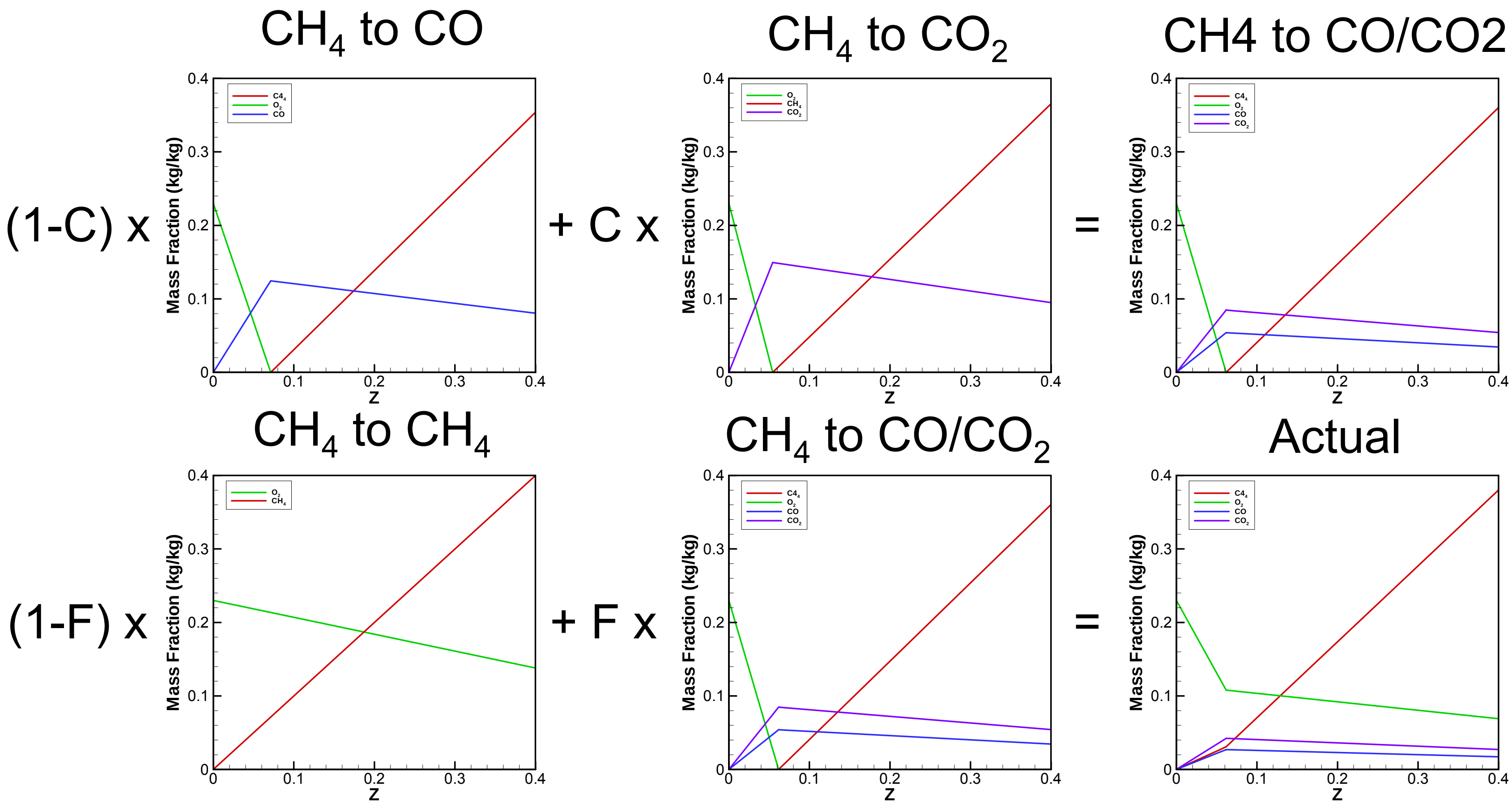
Mass of unburned fuel

Mass of fuel converted to CO and associated products

Mass of fuel converted to CO_2 and associated products

$$Z_1 + Z_2 + Z_3 = Z$$

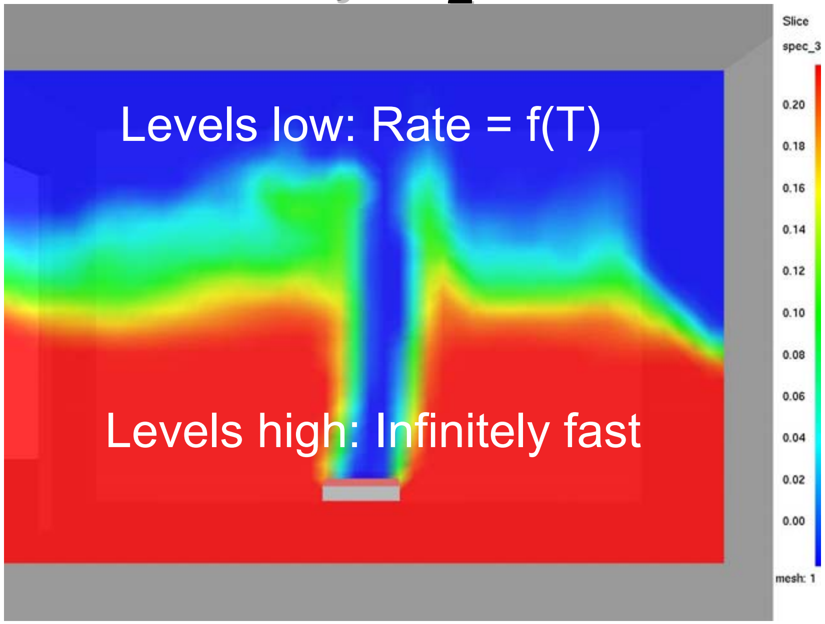
Three-parameter State Relations



F = Degree of completion of combustion (F=0.5)
C = Degree of conversion of CO (C=0.5)
for clarity, N_2 and H_2O have been omitted

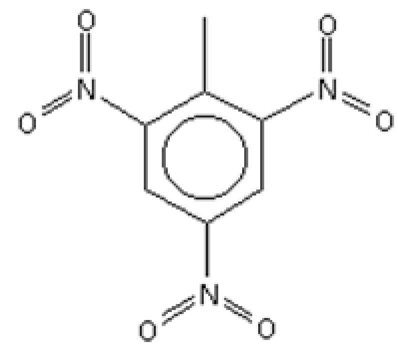
Reaction Kinetics

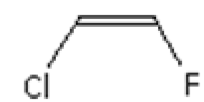
- Reaction 1: Fuel + $O_2 \rightarrow CO + H_2O$
  - Infinitely fast, T vs. O_2
- Reaction 2: $CO + O_2 \rightarrow CO_2$
  - Infinitely fast
  - Base on nearby O_2 levels



&REAC for Mixture Fraction

- FDSv4
  - Specify ideal molar stoichiometry and yields for minor species
  - Not easy to deal with fuels containing elements other than C,H, and O.
- FDSv5
  - Specify the fuel molecule
  - Specify the yields of minor products
  - Heat of combustion
    - actual: reflects minor products
    - ideal: FDS corrects to account for minor products





&REAC for Finite Rate

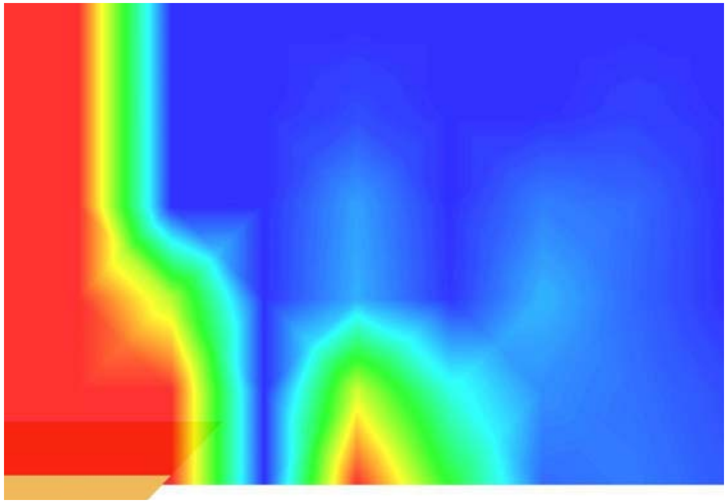
$$CH_4 + 1.5\,O_2 \rightarrow CO + 2\,H_2O \qquad \frac{d[CH_4]}{dt} = -A_1[CH_4]^{-0.3}[O_2]^{1.3}e^{-E_{a,1}/RT}$$

$$CO + 0.5\,O_2 \rightarrow CO_2 \qquad \frac{d[CO]}{dt} = -A_2[CO]^{1}[O_2]^{0.25}[H_2O]^{0.5}e^{-E_{a,2}/RT}$$

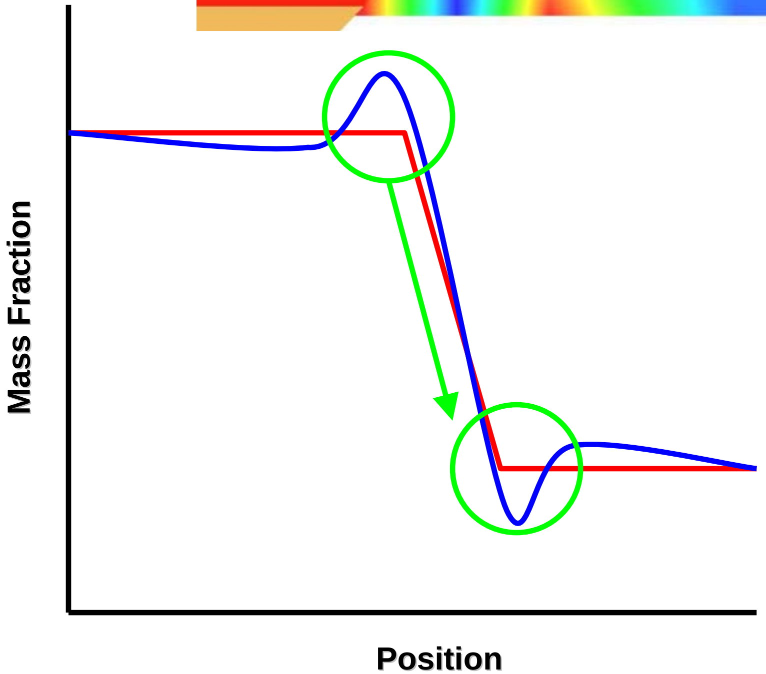
- FDSv4
  - Above was not possible
  - One reaction
  - Rate exponents the same as stoichiometry
- FDSv5
  - NU() : Reaction stoichiometry
  - N() : Arrhenius exponents. Now possible to specify a reaction rate dependence that includes non-participating species

Flux Correction

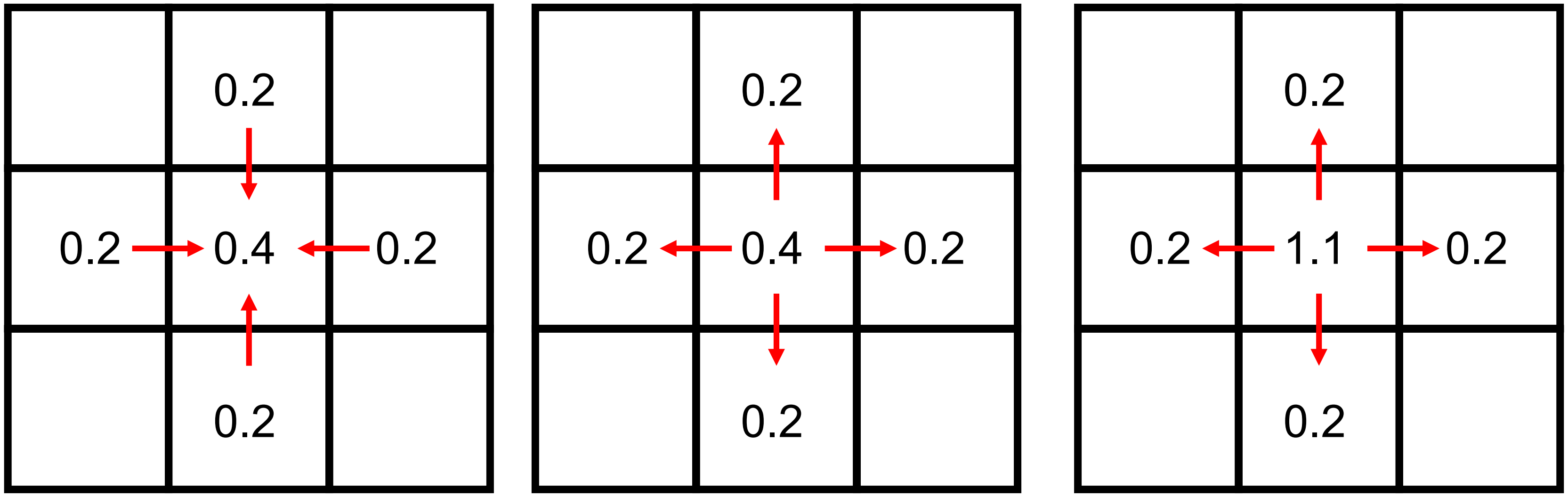
- “Ringing” in solution of species transport equation in regions of high gradients.



Want an approach to shift the mass in a conserving manner to “correct” the solution. This will increase numerical diffusion but prevent non-physical solutions (for example negative species mass fractions)



Flux Correction



Correction needed:
Higher than surroundings with influx

No correction needed:
Higher than surroundings with outflux

Correction needed:
Higher than absolute limit

Mass flux direction

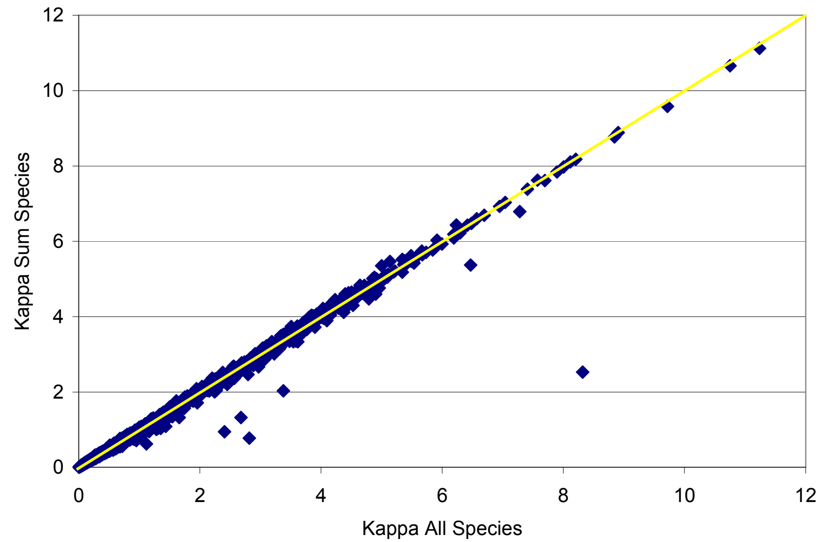
0.2 Mass fraction Z_1

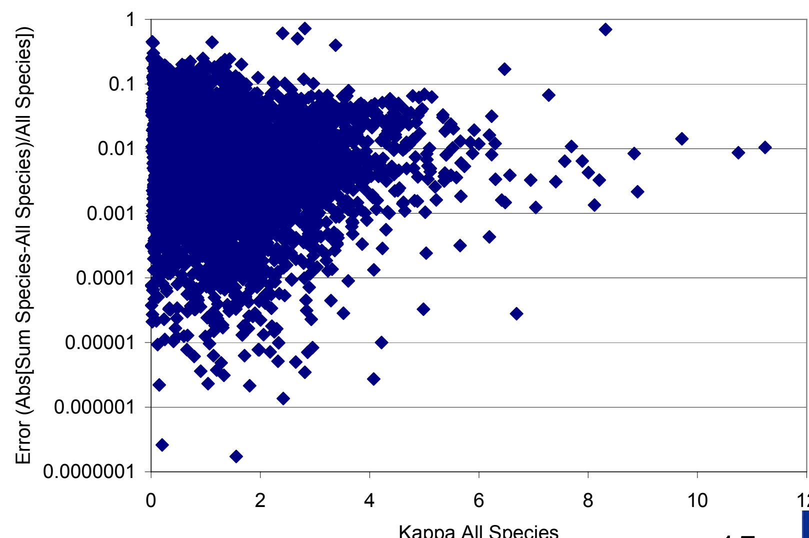
Radiation

- FDS v2-v4
  - used RADCAL (Grosshandler, 1993) to compute an absorbtivity lookup table: $\kappa(Z,T)$
  - Non-MF computations could only have fixed background κ.
  - FVM solver for transport (Hostikka)
- FDS v5
  - $\kappa(Z,T)$ becomes $\kappa(Z_1, Z_2, Z_3,T)$. Time consuming to initialize and costly memory storage for a similar lookup table
  - Wish to generate κ non-mixture fraction computations
  - Still use FVM solver

Radiation

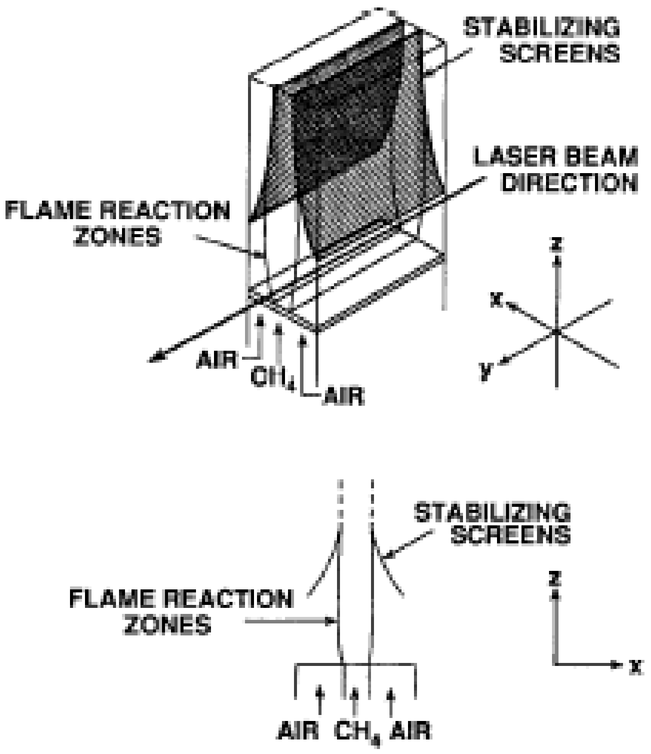
- Compare random states of combustion (fuel, species, temperature, path) for the absorptivity of all species to sum for each species at that mass fraction
  - 96 % summed values within 10 % of combined values
  - 99.5 % within 20 %
  - Outliers are predominately cold with very high levels of soot (not likely to occur in a typical simulation)
- FDSv5
  - Computes a table of $\kappa(Y,T)$ and $\kappa(I,J,K)$ is computed by a weighted sum
  - Can now generate $\kappa(I,J,K)$ for finite rate



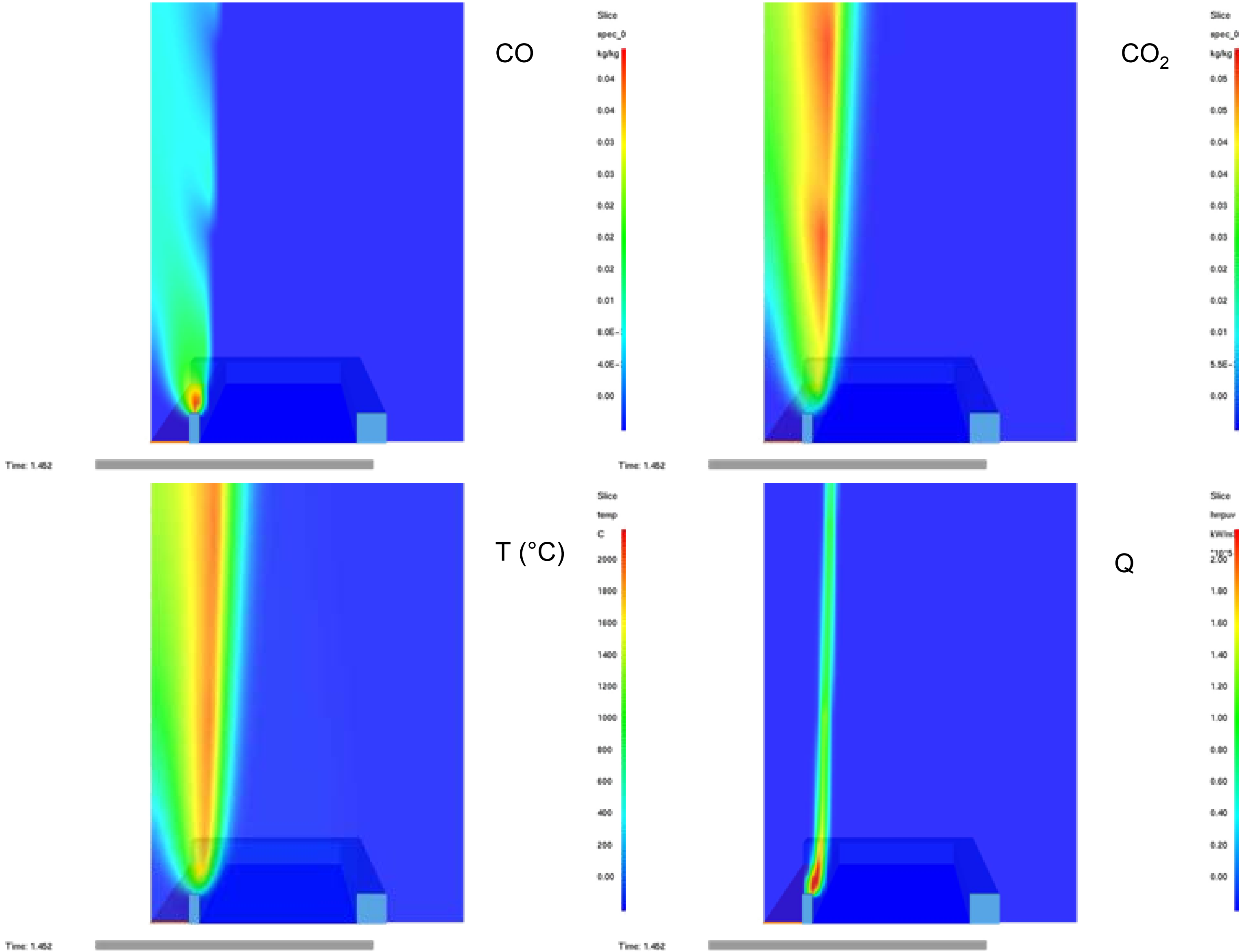


Wolfhard-Parker Slot Burner
(Norton, Smyth, Miller, Smooke 1992)

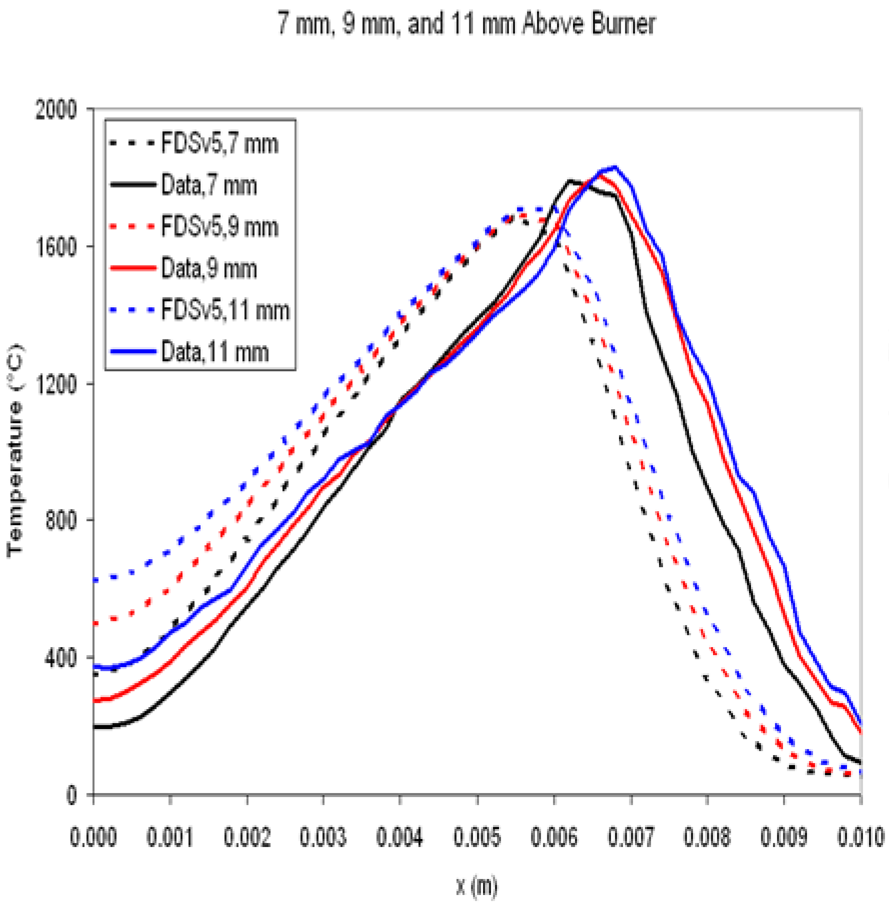
- 2D laminar, methane-air, diffusion flame
- Measured temperature and many major and minor species at elevations near the burner surface

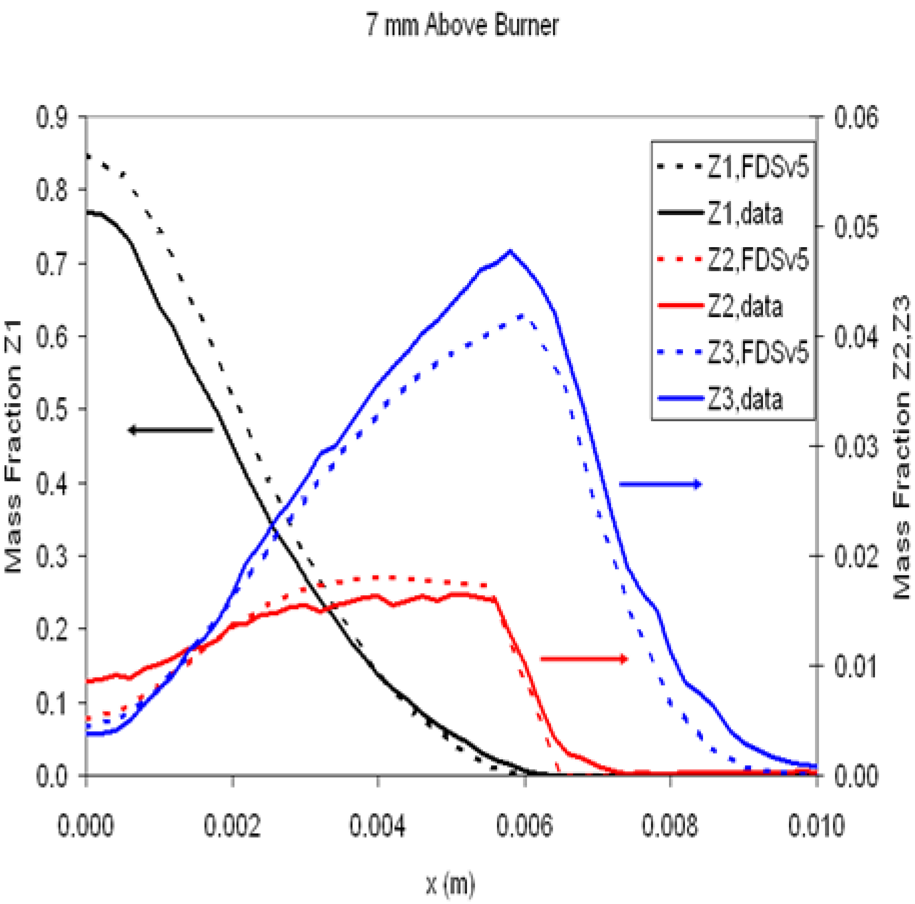


Slot Burner – FDS v5



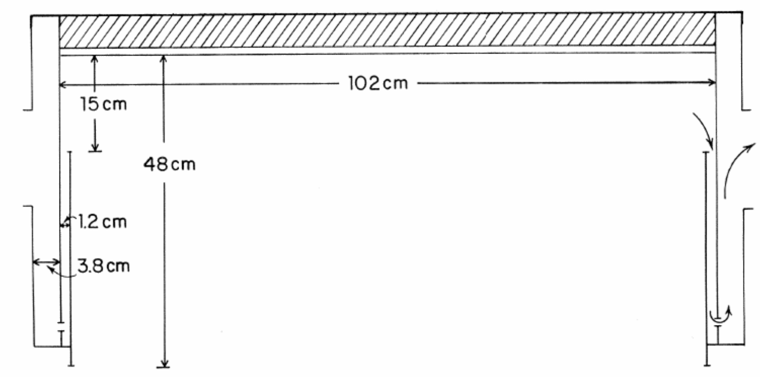
Comparison with Data

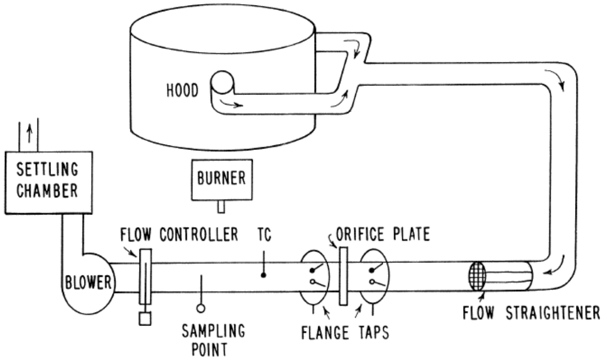




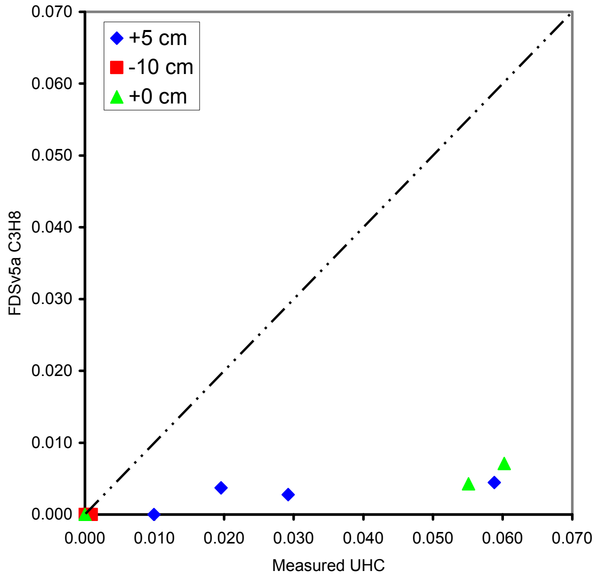
Beyler Hood

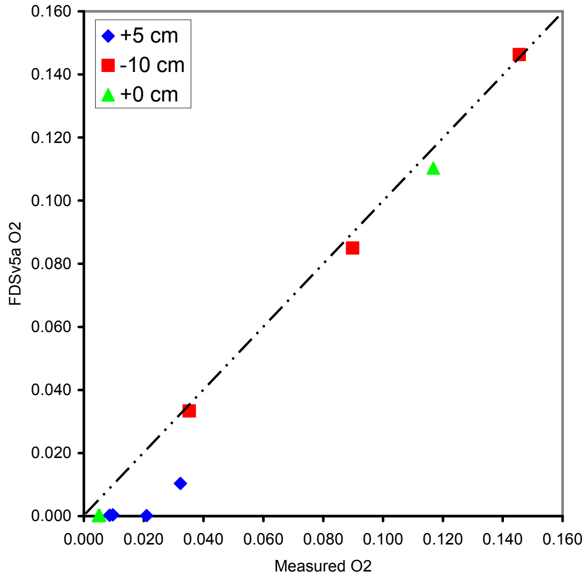
- Adjustable height burner located beneath a hood
- Varied distance from hood lip to burner surface, burner diameter, fuel, and fire size
- Hood exhaust rate manually controlled to prevent spill from the hood lip
- Measured gas concentrations in the exhaust duct

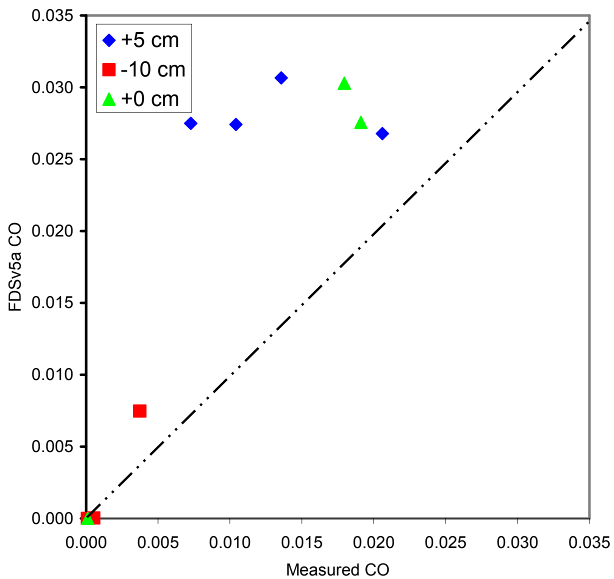


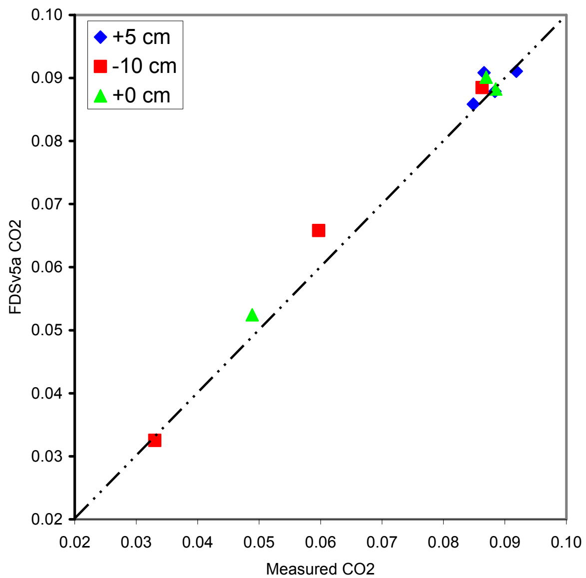


Results


0.070
0.060
0.050
0.040
0.030
0.020
0.010
0.000
FDSv5a C3H8
+5 cm
-10 cm
+0 cm
0.000 0.010 0.020 0.030 0.040 0.050 0.060 0.070
Measured UHC

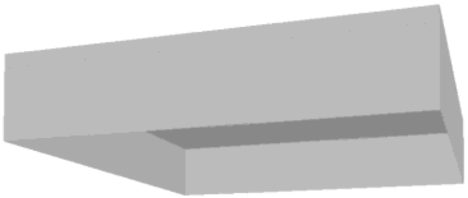

0.160
0.140
0.120
0.100
0.080
0.060
0.040
0.020
0.000
FDSv5a O2
+5 cm
-10 cm
+0 cm
0.000 0.020 0.040 0.060 0.080 0.100 0.120 0.140 0.160
Measured O2

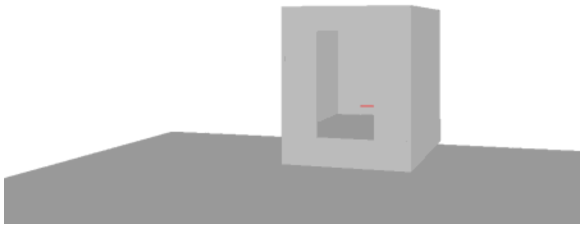

0.035
0.030
0.025
0.020
0.015
0.010
0.005
0.000
FDSv5a CO
+5 cm
-10 cm
+0 cm
0.000 0.005 0.010 0.015 0.020 0.025 0.030 0.035
Measured CO

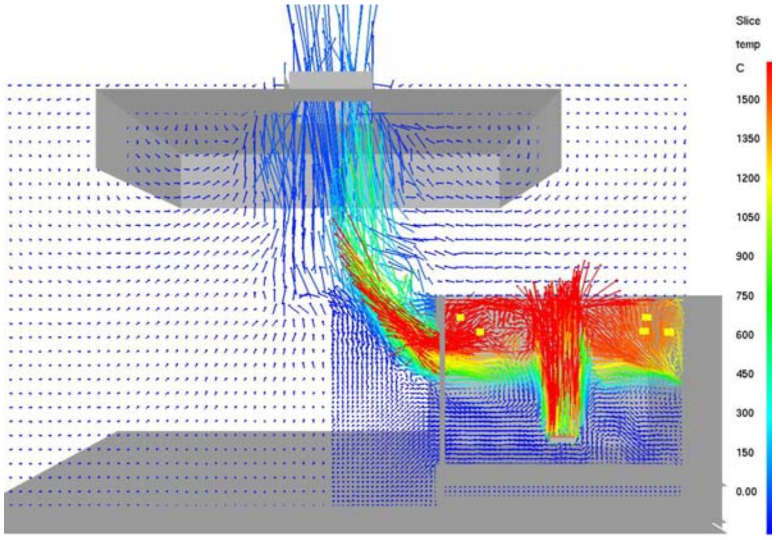

0.10
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
FDSv5a CO2
+5 cm
-10 cm
+0 cm
0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.10
Measured CO2

RSE Experiments
(Bryner, Johnsson, Pitts, 1994)

- 40 % of an ISO-9705 room
- Elevated methane burner
- Gas concentration measurements in upper layer at front and back of compartment



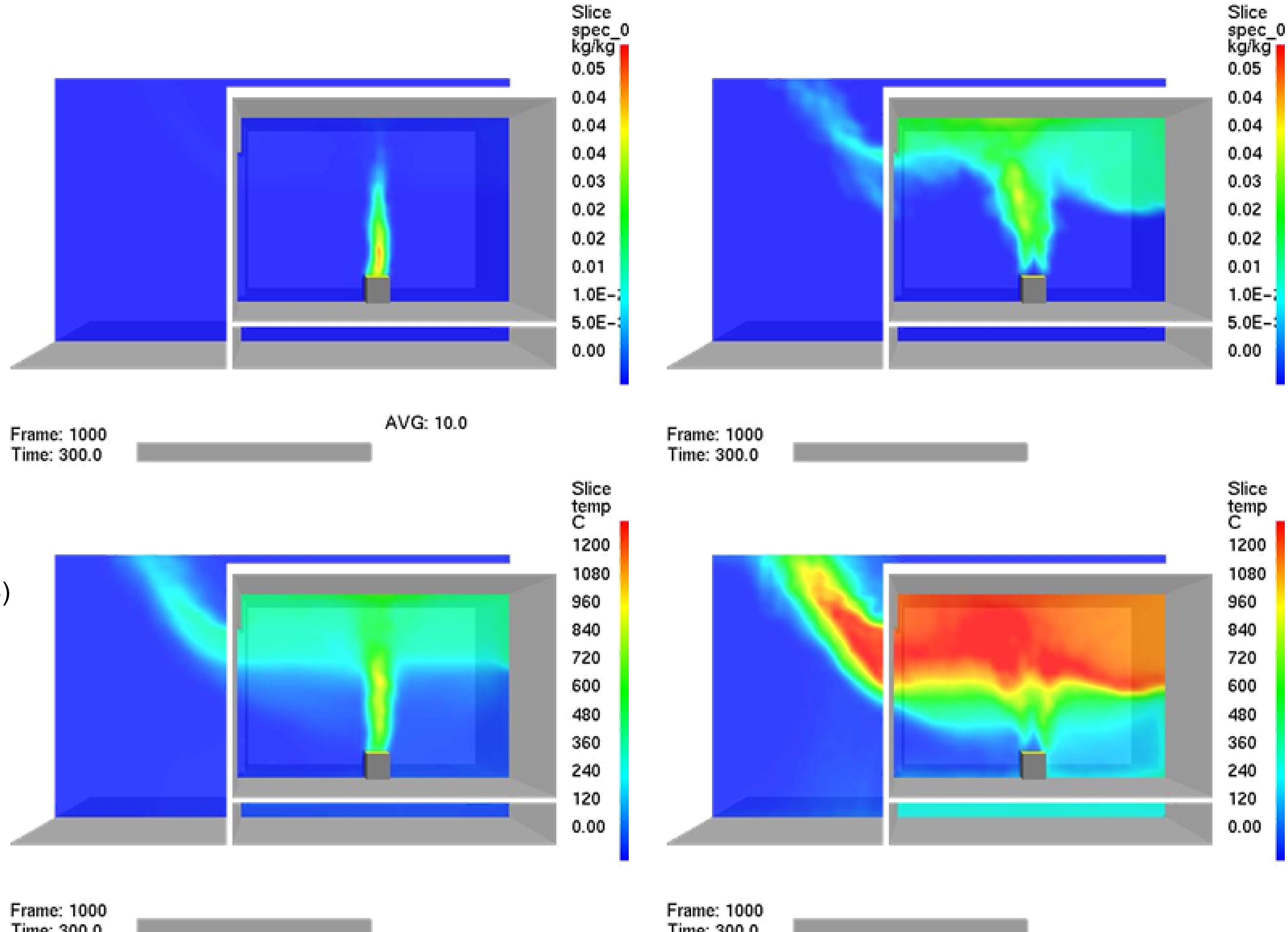




50 kW & 400 kW

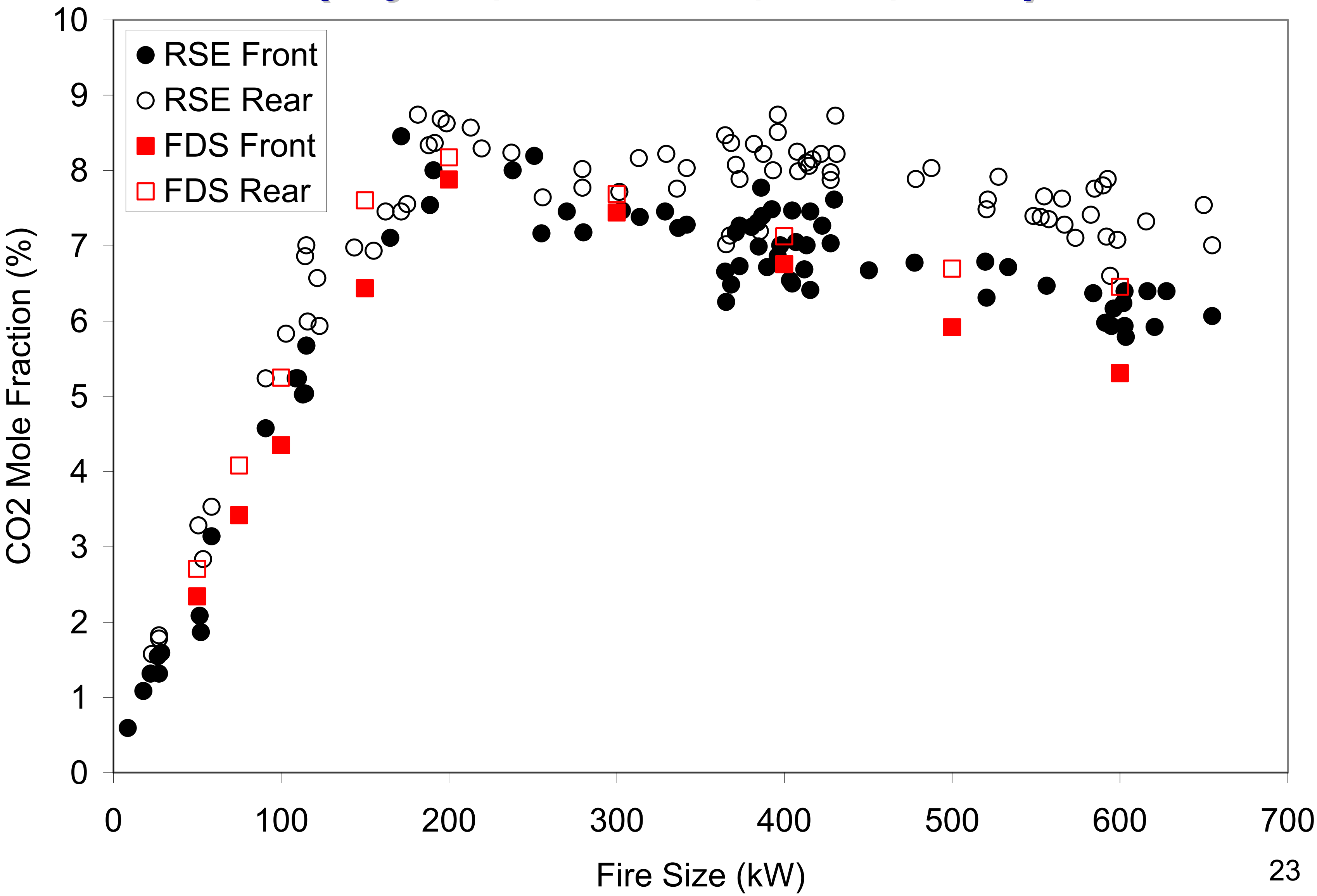
CO

T (°C)



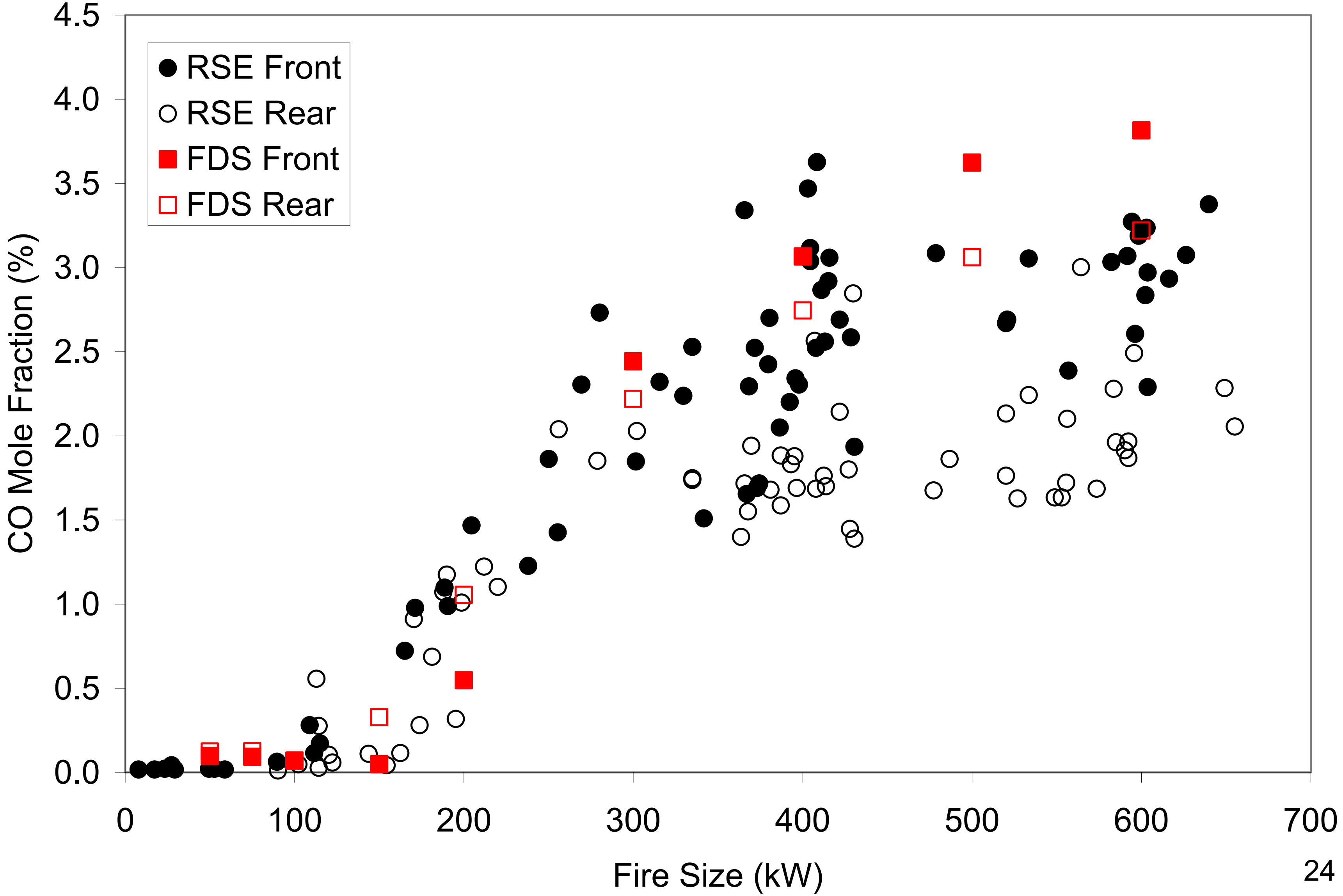
CO_2: FDS v4 + v5 vs. Data

(Bryner, Johnsson, Pitts, 1994)



CO: FDS v4 + v5 vs. Data

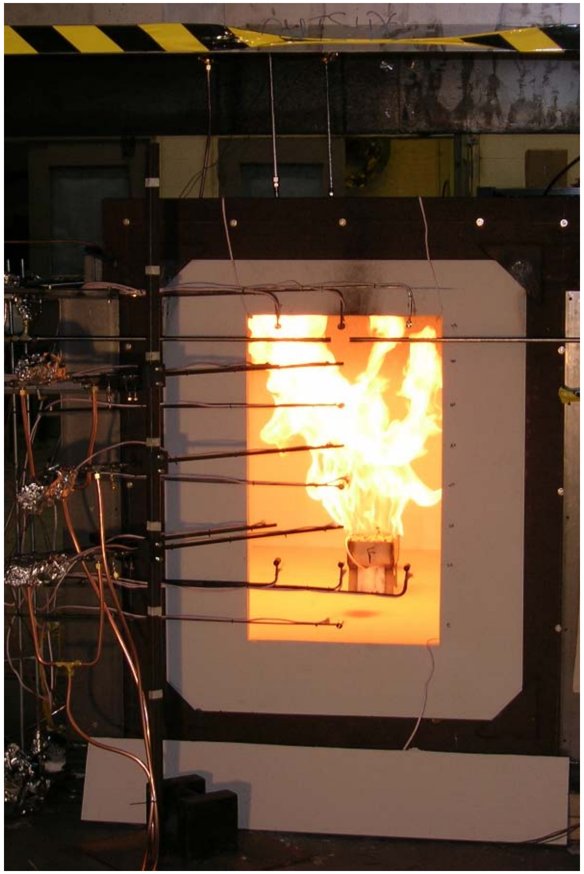
(Bryner, Johnsson, Pitts, 1994)



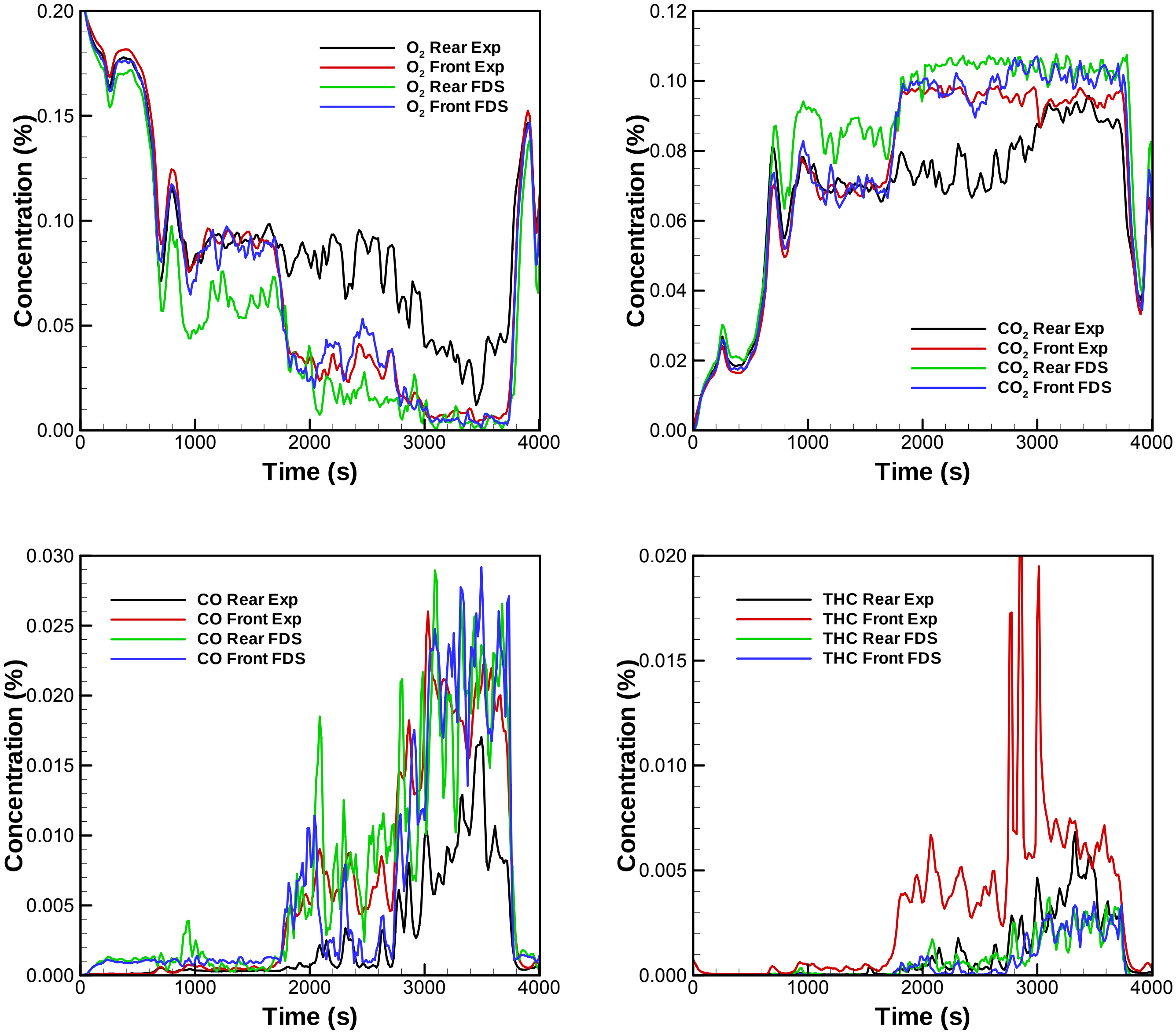
New RSE Tests

(Johnsson, Bundy, Hamins)

- Currently conducting testing using RSE
- Primary goal to reduce dataset uncertainties for use as FDS validation
- Gaseous, liquid pool, and liquid spray fuels

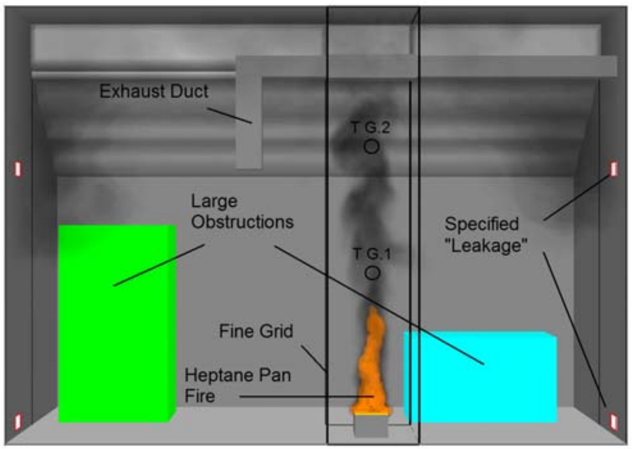


RSE Test #7 - Heptane

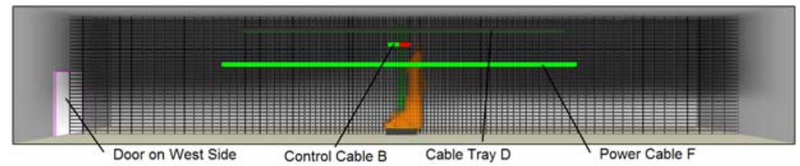


US NRC Validation Cases

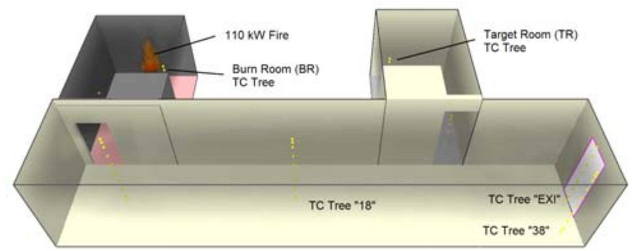
VTT, Finland



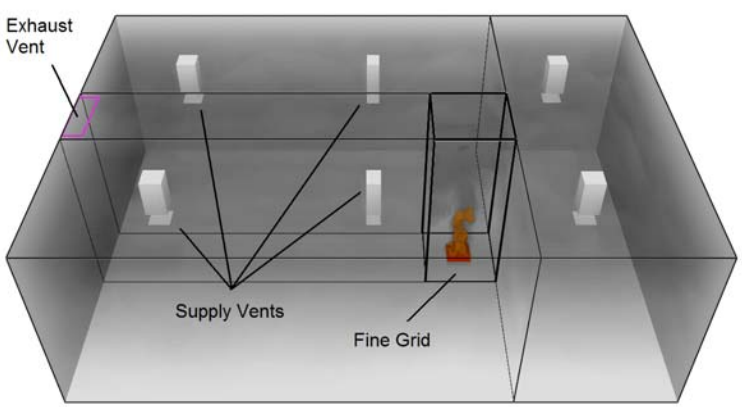
NIST, USA



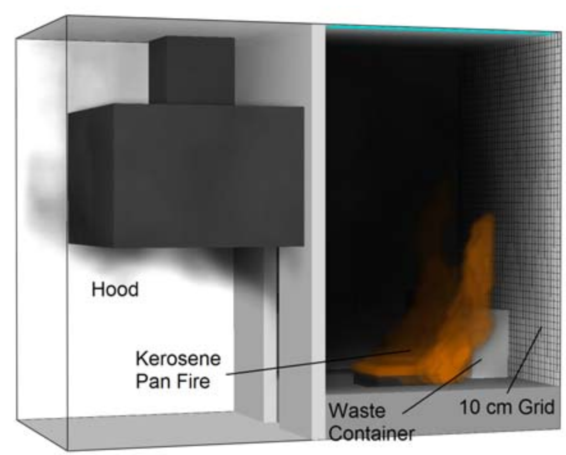
NBS, USA



Sandia/FM (USA)

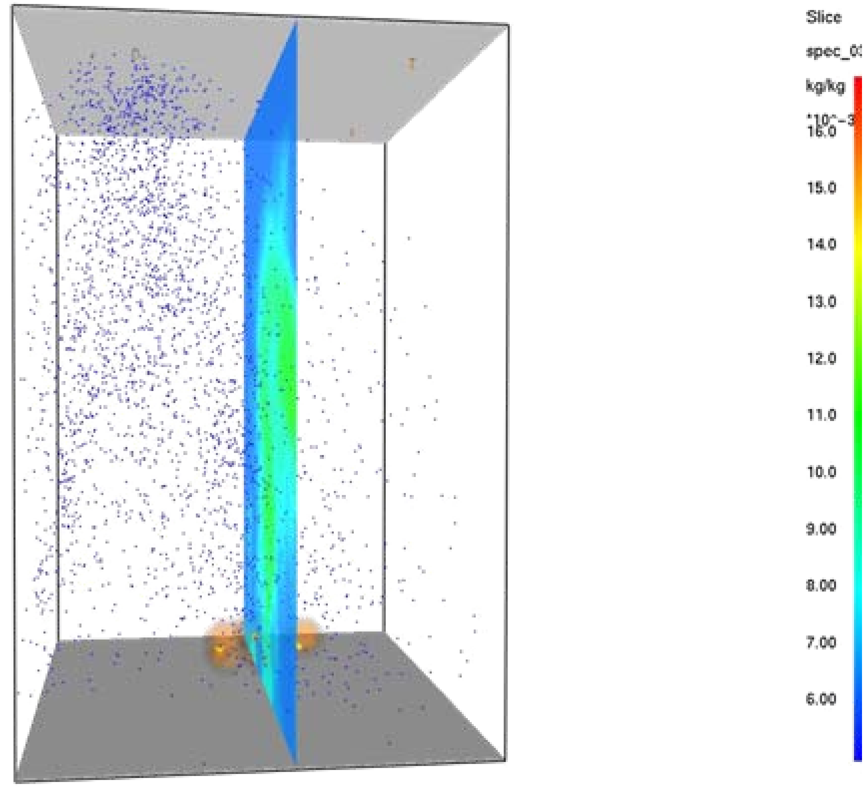


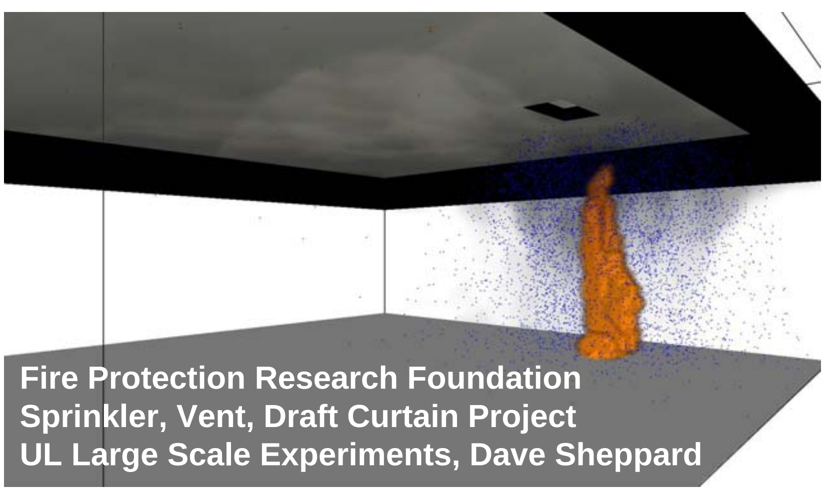
iBMB, Germany



Water + Fuel Sprays

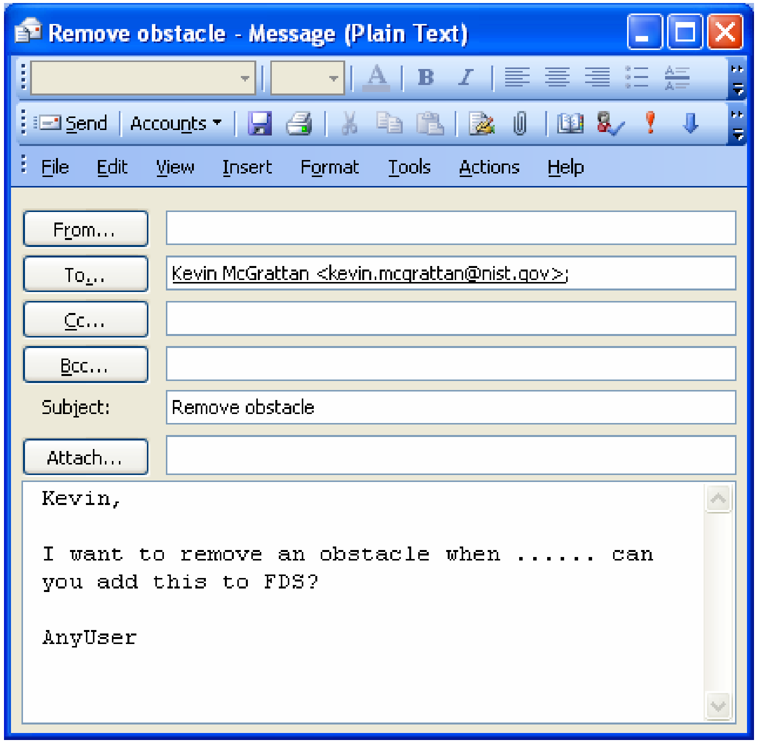
- New droplet type structures
- Allow for simultaneous fuel and water sprays
- Each particle type is assigned its own outputs




Fire Protection Research Foundation
Sprinkler, Vent, Draft Curtain Project
UL Large Scale Experiments, Dave Sheppard

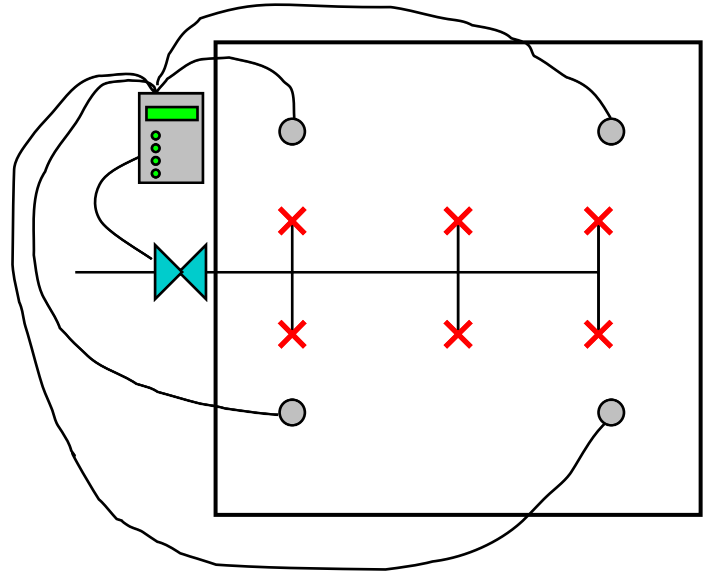
Control Functions

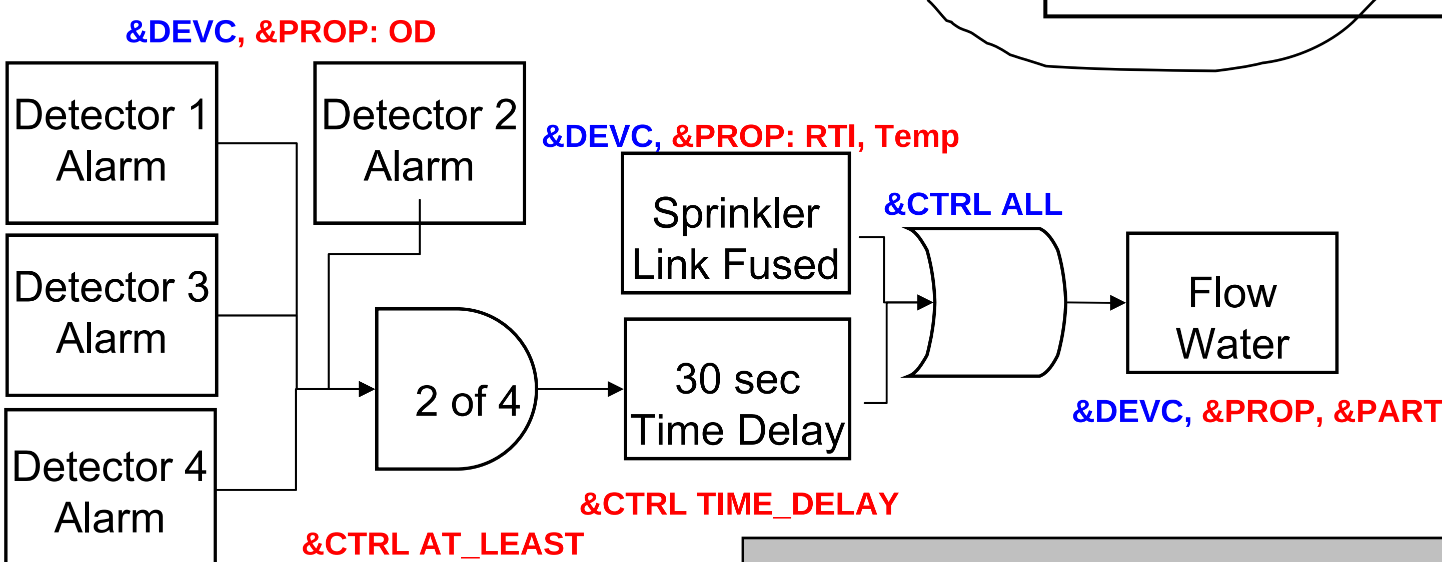
- Added the ability for any point measurement device to add/remove and obstacle, open/close a vent, start/stop a sprinkler.
- Added the ability to do additional logic with a control function input: &CTRL
  - ANY (1 of X), ALL (X of X), ONLY (N of X), AT_LEAST (N or greater of X)
  - TIME_DELAY: wait a period of time from an event
  - RESTART, KILL: dump restart, stop execution
  - CUSTOM: define on/off behavior as a function of a real valued input



Pre-Action Sprinkling

- 2 of 4 detectors open valve
- 30 s to flood pipe
- must also have open head



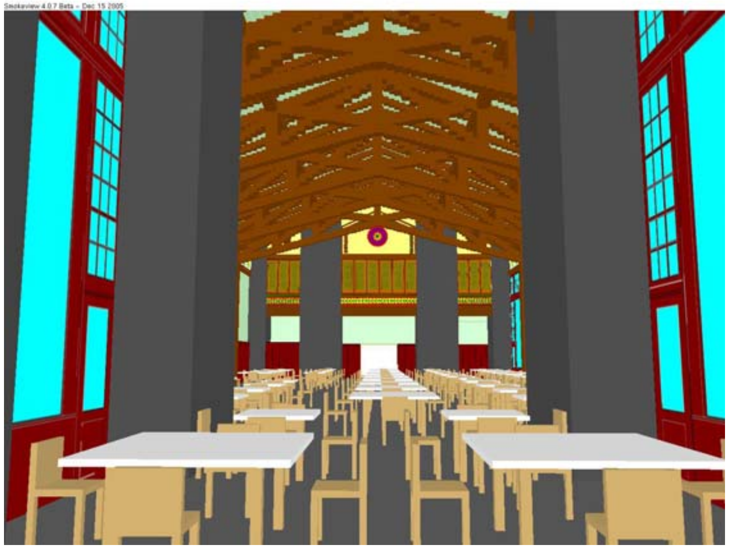


DEFINE FOR EACH SPRINKLER OR DETECTOR

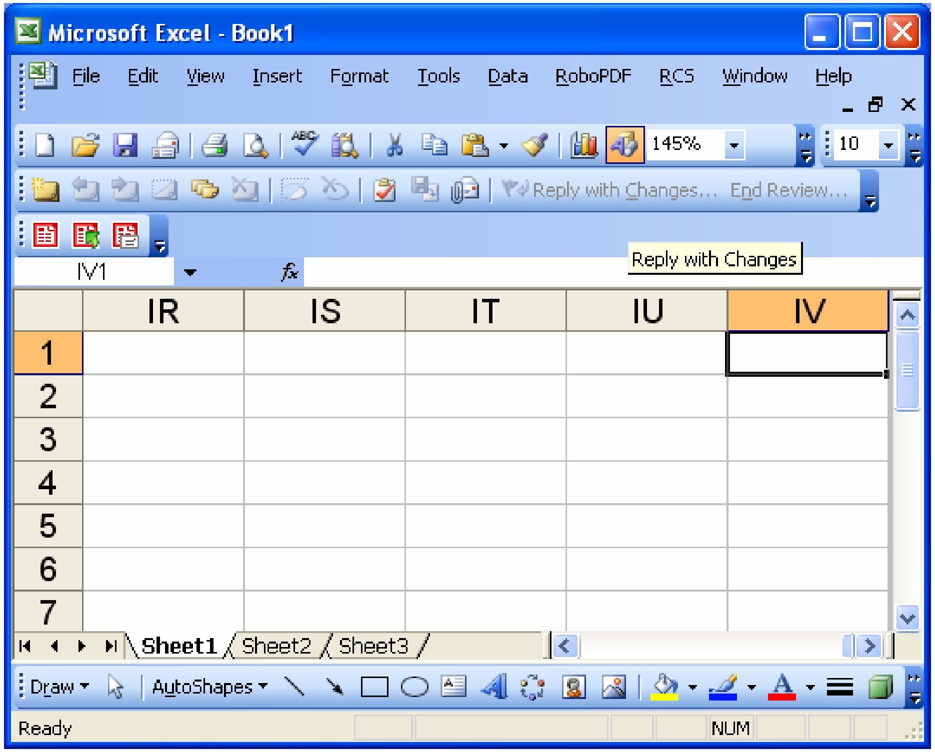
DEFINE ONCE

Smoke Detection

- Added two new smoke detector models:
  - linear beam detector. Specify beam source/target locations and obscuration for alarm
  - Aspiration detector: Specify sampling locations, flowrate, transport time, and obscuration for alarm



%^$!!! 256 Column Limit



- csv output files will now automatically split into mutiple files to avoid exceeding Excel column limit. Disable with COLUMN_DUMP_LIMIT flag on &DUMP

Outputs

- FDSv4 - Each type (SLCF, PL3D, THCP, etc) computed is own quantities. Not all possible outputs were available for each type (only a handful allowed for ISOF).
- FDSv5 – Each type now calls the same DEVC updating routine to determine either a single point, a plane, or a volume.

Table 4.3: Summary of all Output Quantities

Output QUANTITY	Symbol	Units	File Type
ABSORPTION_COEFFICIENT	κ	1/m	D,I,P,S
ADIABATIC_SURFACE_TEMPERATURE	$T_{\rm AST}$ (see Sec. 4.16.13)	°C	B,D
BURNING_RATE	$\dot{m}''_f$	kg/m²/s	B,D
carbon dioxide	$X_{CO_2}(Z)$	mol/mol	D,I,P,S
carbon monoxide	$X_{CO}(Z)$	mol/mol	D,I,P,S
CONVECTIVE_FLUX	$\dot{q}''_c$ (Section 4.16.12)	kW/m²	B,D
DENSITY	ρ	kg/m³	D,I,P,S
DIVERGENCE	$\nabla \cdot \mathbf{u}$	s^{-1}	D,I,P,S
DROPLET_DIAMETER	$2r_d$	μm	PA
DROPLET_VELOCITY	$\lvert\mathbf{u}_d\rvert$	m/s	PA
DROPLET_TEMPERATURE	T_d	°C	PA
DROPLET_MASS	m_d	kg	PA
DROPLET_AGE	t_d	s	PA
DROPLET_FLUX_X	$\dot{m}''_w$	kg/m²/s	P,S
DROPLET_FLUX_Y	$\dot{m}''_w$	kg/m²/s	P,S
DROPLET_FLUX_Z	$\dot{m}''_w$	kg/m²/s	P,S
extinction coefficient	K (Section 4.16.9)	1/m	D,I,P,S
fuel	$X_F(Z)$	mol/mol	D,I,P,S
GAUGE_HEAT_FLUX	See Section 4.16.12	kW/m²	B,D
H	$H = \lvert\mathbf{u}\rvert^2/2 + \tilde{p}/\rho_0$	(m/s)²	D,I,P,S
HEAT FLOW	See Section 4.16.15	kW	D
HEAT_FLUX	See Section 4.16.12	kW/m²	B,D
HRR	$\int \dot{q}''' \, dV$	kW	D
HRRPUV	$\dot{q}'''$	kW/m³	D,I,P,S
INCIDENT_HEAT_FLUX	See Section 4.16.12	kW/m²	B,D
INSIDE_WALL_TEMPERATURE	See Section 4.16.3	°C	D
LAYER HEIGHT	See Section 4.16.10	m	D
LOWER TEMPERATURE	See Section 4.16.10	°C	D
MASS FLOW	See Section 4.16.15	kg/s	D

B=BNDF, D=DEVC, I=ISOF, P=PL3D, PA=PART, S=SLCF

CFD: Colorful Fluid Dynamics

- Motivated by laziness
  - Tedious to determine RGB values for non-primary colors.
  - Most graphics programs do 0-255 integer and FDSv4 did 0.-1. real
- In FDSv5
  - RGB is now 0 to 255 integer (don't have to convert to real)
  - 500+ colors names defined